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Institute for Scientific Computing Research

Annual Report: Fiscal Year 2004

Collaborating with Academia

UNIVERSITY RELATIONS PROGRAM

The University Relations Program (URP) encourages collaborative research between Lawrence Livermore National Laboratory (LLNL) and the University of California campuses. The Institute for Scientific Computing Research (ISCR) actively participates in such collaborative research, and this report details the Fiscal Year 2004 projects jointly served by URP and ISCR. For a full discussion of all URP projects in FY 2004, please request a copy of the URP FY 2004 Annual Report by contacting

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UCRL-TR-133866-04

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Director's Report

Large-scale scientific computation and all of the disciplines that support and help to validate it have been placed at the focus of Lawrence Livermore National Laboratory (LLNL) by the Advanced Simulation and Computing (ASC) program of the National Nuclear Security Administration (NNSA) and the Scientific Discovery through Advanced Computing (SciDAC) initiative of the Office of Science of the Department of Energy (DOE). The maturation of computational simulation as a tool of scientific and engineering research is underscored in the November 2004 statement of the Secretary of Energy that, "high performance computing is the backbone of the nation's science and technology enterprise."

LLNL operates several of the world's most powerful computers—including today's single most powerful—and has undertaken some of the largest and most compute-intensive simulations ever performed. Ultrascale simulation has been identified as one of the highest priorities in DOE's facilities planning for the next two decades. However, computers at architectural extremes are notoriously difficult to use efficiently. Furthermore, each successful terascale simulation only points out the need for much better ways of interacting with the resulting avalanche of data. Advances in scientific computing research have, therefore, never been more vital to LLNL's core missions than at present. Computational science is evolving so rapidly along every one of its research fronts that to remain on the leading edge, LLNL must engage researchers at many academic centers of excellence. In Fiscal Year 2004, the Institute for Scientific Computing Research (ISCR) served as one of LLNL's main bridges to the academic community with a program of collaborative subcontracts, visiting faculty, student internships, workshops, and an active seminar series.

The ISCR identifies researchers from the academic community for computer science and computational science collaborations with LLNL and hosts them for short- and long-term visits with the aim of encouraging long-term academic research agendas that address LLNL's research priorities. Through such collaborations, ideas and software flow in both directions, and LLNL cultivates its future workforce. The Institute strives to be LLNL's "eyes and ears" in the computer and information sciences, keeping the Laboratory aware of and connected to important external advances. It also attempts to be the "feet and hands" that carry those advances into the Laboratory and incorporates them into practice. ISCR research participants are integrated into LLNL's Computing and Applied Research (CAR)

Department, especially into its Center for Applied Scientific Computing (CASC). In turn, these organizations address computational challenges arising throughout the rest of the Laboratory. Administratively, the ISCR flourishes under LLNL's University Relations Program (URP). Together with the other five institutes of the URP, it navigates a course that allows LLNL to benefit from academic exchanges while preserving national security. While it is difficult to operate an academic-like research enterprise within the context of a national security laboratory, the results declare the challenges well met and worth the continued effort.

Fiscal year 2004 was the fifth full year under Acting Director David Keyes. Keyes, the Fu Foundation Professor of Applied Mathematics at Columbia University and an ISCR faculty participant since October 1997, dedicated one-third of his time to the technical program of the ISCR. James McGraw continued as the Deputy Director of the ISCR, and Linda Becker as the Institute Administrator. Paula Ashley, Pamela Mears, and Char

Paulo logistically supported the large visitor and summer programs of the ISCR.

The ISCR continues to have a small contingent of research staff members within its organization. Three ISCR staff—Nelson Max, Garry Rodrigue, and Rao Vemuri—hold joint appointments as professors at the University of California, Davis and senior researchers at LLNL. In addition, the ISCR hosted eight post-doctoral staff: Alison Baker, David Buttler, Tzanio Kolev, Shawn Newsam, Stefan Nilsson, Dan Reynolds, Megan Thomas, and Qing Yi. Finally, the ISCR served as the host for 10 students (listed in Table 1) on a Student-Employee Graduate Fellowship (SEGRF). This fellowship enables students to work with LLNL researchers half-time while pursuing their PhDs.

The ISCR enables substantial interactions between academia and LLNL staff through consultants and participating guests. Consulting agreements are vehicles for permitting academics to interact with LLNL in a compensated fashion. Consultants may serve on review committees, present short courses, and visit LLNL periodically for

Table 1. Students on a Student-Employee Graduate Fellowship (SEGRF).

Name	University	LLNL Advisor(s)	Time at LLNL
Peer-Timo Bremer	University of California, Davis	Dan Laney	June 12, 2002 – Aug. 6, 2004
Sam Brockington	University of California, Davis	Garry Rodrigue & Dave Hwang	Oct. 8, 2001 – Aug. 31, 2006
Paul Castellucci	Stanford University	Rose McCallen	Oct. 13, 2003 – Jan. 31, 2005
Aaron Fisher	University of California, Davis	Garry Rodrigue	July 1, 2002 – June 30, 2006
Benjamin Gregorski	University of California, Davis	Mark Duchaineau	June 25, 2001 – Aug. 13, 2004
Jeff Hagelberg	Purdue University	Paul Amala	Sept. 22, 2003 – Sept. 25, 2004
Aaron Herrnstein	University of California, Davis	Michael Wickett	Mar. 26, 2004 – Mar. 31, 2004
Andrew Nonaka	University of California, Davis	David Trebotich	Oct. 1, 2003 – Sept. 30, 2007
Rob Rieben	University of California, Davis	Garry Rodrigue	Oct. 2, 2000 – Oct. 1, 2004
Joshua Senecal	University of California, Davis	Mark Duchaineau	Nov. 1, 2001 – Oct. 31, 2005

Table 2. Nine ISCR consultants for FY 2004.

Consultant	Affiliation	LLNL Contact
Randolph Bank	University of California, San Diego	Rob Falgout
Achiezer Brandt	University of California, Los Angeles	Rob Falgout
Gene Golub	Stanford University	Edmond Chow
Anne Greenbaum	University of Washington	Peter Brown
Heinz-Otto Kreiss	University of California, Los Angeles	Lori Diachin & Bill Henshaw
Thomas Manteuffel	University of Colorado	Rob Falgout & Peter Brown
Stephen McCormick	University of Colorado	Rob Falgout & Peter Brown
Linda Petzold	University of California, Santa Barbara	Carol Woodward & Radu Serban
Homer Walker	Worcester Polytech Institute	Peter Brown

technical meetings. All consultants have a specific LLNL technical point of contact for overseeing their interactions. Table 2 lists the nine ISCR consultants for FY 2004.

Participating Guests are researchers from academia or industry that need intermittent access to LLNL staff and facilities. This status permits an appropriate security clearance and the ability to quickly arrange for on-site visits with LLNL staff over a period of one month to two years. Table 3 lists ISCR's 38 participating guests for FY 2004.

The pages of this annual report summarize the activities of the faculty members, postdoctoral researchers, students, and guests from industry and other laboratories who participated in LLNL's computational mission under the auspices of the ISCR during FY 2004. These activities, which are further detailed in the accompanying CD-ROM, fall

Table 3. ISCR's 38 participating guests for FY 2004.

Guest	Affiliation	LLNL Contact	Dates
Marian Brezina	University of Colorado	Rob Falgout	Dec. 1, 2000 – Nov. 30, 2004
Zhiqiang Cai	Purdue University	Charles Tong	Sept. 8, 2003 – Sept. 7, 2005
Praveen Chandramohan	Oak Ridge National Laboratory	Terence Critchlow	Nov. 7, 2003 – May. 6, 2004
Alok Choudhary	Northwestern University	Terence Critchlow	Sept. 15, 2003 – Sept. 13, 2005
Jennifer Dacles-Mariani	University of California, Davis	Garry Rodrigue	Sept. 1, 2003 – Aug. 30, 2005
Hans de Sterck	University of Colorado, Boulder	Rob Falgout	Oct. 1, 2003 – Sept. 30, 2004
Branden E. Fitelson	University of California, Berkeley	Terence Critchlow	Aug. 9, 2004 – Aug. 8, 2005
Franz Franchetti	Carnegie Mellon University	Kim Yates	June 4, 2004 – June 3, 2005
Alejandro Garcia	San Jose State University	Richard Hornung	Oct. 12, 2001 – Oct. 10, 2004
William Charles Gear	Princeton University	Steve Lee	Sept. 21, 2004 – Sept. 20, 2005
Matthew R. Gibbons	U.S. Airforce Academy	Bill Bateson	Aug. 9, 2004 – Aug. 8, 2005
Bernd Hamann	University of California, Davis	Mark Duchaineau	Aug. 9, 2004 – Aug. 8, 2005
Alan Hindmarsh	LLNL (retired)	Carol Woodward	Oct. 1, 2002 – Sept. 29, 2004
Martin Isenburg	University of North Carolina	Terence Critchlow	Nov. 4, 2003 – Nov. 3, 2004
Ken Joy	University of California, Davis	Mark Duchaineau	June 4, 2003 – June 3, 2005
Ramya Krishnamurthy	Oak Ridge National Laboratory	Terence Critchlow	Nov. 7, 2003 – Nov. 6, 2004
Johannes K. Kraus	University of Loeben	Van Henson	Nov. 30, 2002 – Sept. 28, 2004
Raytcho Lazarov	Texas A&M University	Panayot Vassilevski	Aug. 31, 2002 – Aug. 28, 2005
Oren Livne	Stanford University	Van Henson	Sept. 15, 2003 – Sept. 14, 2004
Bertram Ludaescher	San Diego Supercomputer Center	Terence Critchlow	Sept. 1, 2001 – Oct. 26, 2004
Jeannee Martin	LLNL (retired)	Bronis de Supinski	March 20, 2004 – March 19, 2005
Sally McKee	Cornell University	Bronis de Supinski	Oct. 14, 2001 – Oct. 13, 2004
Esmond Ng	Lawrence Berkeley National Laboratory	Edmond Chow	May 12, 2003 – May 11, 2004
Beth Ong	LLNL	Van Henson	Aug. 1, 2001 – Dec. 1, 2004
Peter Pacheco	University of San Francisco	Pat Miller	Aug. 9, 2004 – Aug. 8, 2005
Joseph E. Pasciak	Texas A&M University	Panayot Vassilevski	July 1, 2002 – June 29, 2005
Christoph Pflaum	Universität Erlangen-Nürnberg	Rob Falgout	Aug. 25, 2003 – Aug. 24, 2004
Elbridge Gerry Puckett	University of California, Davis	Louis Howell	June 30, 2003 – June 29, 2004
Markus Pueschel	Carnegie Mellon University	Kim Yates	April 14, 2003 – May 18, 2005
Ulrich Ruede	Universität Erlangen-Nürnberg	Rob Falgout	Aug. 15, 2000 – July 29, 2004
Paul E. Saylor	University of Illinois	Steve Lee	Aug. 22, 2004 – Aug. 21, 2005
Martin Schultz	Cornell University	Bronis de Supinski	March 1, 2003 – Dec. 30, 2004
M. Alex Schweitzer	Universität Bonn	Rob Falgout	Nov. 17, 2003 – July 22, 2005
Claudio Silva	University of Utah	Randy Frank	May 19, 2003 – June 3, 2004
Lansing Sloan	LLNL (retired)	Pete Eltgroth	June 16, 2004 – June 15, 2005
Christoph W. Ueberhuber	Techische Universität Wien	Kim Yates	March 1, 2003 – Feb. 28, 2004
Beata Winnicka	Argonne National Laboratory	Dan Quinlan	Aug. 15, 2003 – Aug. 14, 2004
Gabriel Wittum	Universität Heidelberg	Rob Falgout	Nov. 17, 2003 – Nov. 16, 2004

under two main themes: sponsored-research activities that stimulate interactions between academia and LLNL staff, and a diverse visitor program that enables both short- and long-term residential stays at LLNL.

ISCR oversees three different types of sponsored-research activities. The University Collaborative Research Program (UCRP), through the ISCR, funded seven research projects during FY 2004 at University of California campuses. These projects supported graduate students working on doctoral thesis research. The faculty principal investigators and students worked closely with an LLNL collaborator. The ISCR also coordinated the funding of 19 research subcontracts to various academic institutions throughout the United States. These contracts are normally funded by programs at LLNL to help address long-term Laboratory requirements. This type of vehicle is also used to fund sabbatical visits to LLNL for three to six months. Eleven faculty members spent at least a portion of their sabbatical leave here during FY 2004. With Laboratory Directed Research and Development (LDRD) funds, the ISCR also funds Exploratory Research in the Institutes (ERI). These research grants are awarded to LLNL staff with the goal of developing ties to academia through co-funded research projects. The ISCR oversaw three such projects in FY 2004. Annual summaries for LDRD projects, UCRP projects, and

Figure 1. ISCR Visitor Program FY1997–FY2004

subcontracts can be found in the next three sections of this document.

In FY 2004, the ISCR continued its tradition of an extensive and diverse Visitor Program. This program includes sabbatical visitors, sponsored workshops, summer students, and various seminars featuring external speakers. Altogether, the ISCR hosted 215 visits from 161 different visitors, an average of more than 4 visits per week. The vast majority (67%) of the visitors were from academia, with 9% from industry, 20% from other federal laboratories, and 4% from non-laboratory-based government institutions. Visitors from outside the United States made up 25% of the total.

The ASC Institute for Terascale Simulation Lecture Series was established in 2000 to enrich the intellectual atmosphere of LLNL's large simulation community through the visits of leaders representing the diverse areas of computation. In FY 2004, we hosted five speakers in this series. The general ISCR seminar series included an additional 65 talks covering a wide spectrum of research areas. Titles of all of these talks can be found in the Seminar Series section of this report, and associated abstracts can be found on the accompanying CD-ROM.

During the summer, ISCR hosted 94 visiting students for a total summer student population of 104, including the SEGRF students in residence year-round. The summer program exposes students to the stimulating and challenging work environment of a national laboratory. Successful candidates are hired as summer employees, assigned individual LLNL mentors, and given specific projects to which they will contribute. The project is appropriate to the student's background and skills, and ranges from programming tasks to original research. The topical coverage of the summer research program broadens each year as computation expands into new scientific areas and as computational tools become more powerful and diverse. Scalable algorithms, radiation transport, genomics, terascale visualization, and computer security are just a handful of topics from last summer's lively hallway conversations at the ISCR. The summer program runs from May to September, with most participants spending 10–12 weeks on site. Project
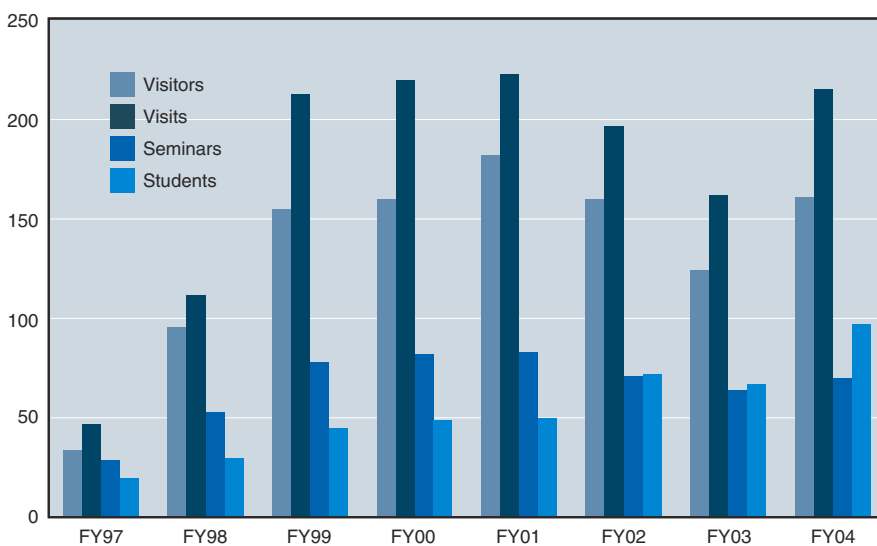
reports for most of the students can be found on the accompanying CD-ROM.

In June, with the advent of our large student summer program and sponsorship from the Defense Programs office of DOE Headquarters, we ramped up our fifth annual Summer Student Lecture Series—three different series on Computational Modeling at the Terascale, Computer Science at the Terascale, and Computer Security. Though the lectures were intended for students, permanent CASC researchers also attended. The 35 lecturers are listed in the Seminar section of this annual report.

Poster presentations were made by 41 ISCR summer students at the LLNL Student Research Symposium in August 2004. The event, held at LLNL's Central Café, attracted local media and scientific staff from across the Laboratory, as well as other students and summer research mentors. Overall, 139 students presented posters, making ISCR's share about 30% of LLNL's total. Topics of the posters ranged from Internet routing patterns to advanced gridding techniques for estuarine flow modeling; from performance modeling tools to wavelet-based compression of radiation opacities; from language interoperability to management of data in petabyte-scale file systems. Students ranged in seniority from community-college first-years to graduate students about to complete their doctorates.

Figure 1 charts the numbers of visitors and seminars over the past eight years. The number of students in residence in FY 2004 increased substantially due to the expansion of the ISCR's responsibility in LLNL's summer programs. CASC scientists mentored 55% of these students. Other LLNL organizations mentoring ISCR summer students were: CADSE, DCOM, EEBI, ICCD, NAIC, NIFE, and PAT. Some of these students elected to spend internships prescribed by their national fellowships at the ISCR, at no direct cost to the Laboratory, including DOE Computational Science Graduate Fellowship (CSGF) holders and Department of Homeland Security (DHS) fellows.

Finally, the ISCR sponsored or co-sponsored 10 scientific workshops in FY 2004. Two of these were hosted locally and exclusively by the ISCR; the rest were in cooperation with other organizations and held off-site. In each case, there is a vital LLNL interest and typically, several LLNL researchers participate. Reports on these workshops appear in a later section of this report.

Most of the raw material of this document comes directly from the visitors and principal investigators of their respective projects. We thank the Technical Information Department, including Alane Alchorn, Arnold Gatilao, Deanna Midtaune, and Al Miguel for their editorial work, Dan Moore for his graphic artistry in producing an easily navigable and visually pleasing document, and Maria Fogle and John Danielson for helping us finalize this document and getting it ready for print.

We hope that you enjoy examining this report on the ISCR's diverse activities in FY 2004. For further information about the Institute, please contact us at the address below. Inquiries about how you might enhance the ISCR program for FY 2005 and beyond are always welcome.

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